Aura Microwave Limb Sounder Lagrangian Trajectory Diagnostics

Users' guide and file description document

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Abstract: This document serves as a users' guide and file description document for the "Lagrangian Trajectory Diagnostic" (LTD) products developed to support scientific studies that use observations from the Aura Microwave Limb Sounder (MLS) launched in 2004. LTD files contain trajectories running from 15-days before to 15-days after each MLS observation. The document briefly describes the generation of these diagnostics, then gives a detailed description of the file format and contents, along with information on where to obtain these files.

Introduction

The Aura Microwave Limb Sounder (MLS) Lagrangian Trajectory Diagnostics (LTDs) are support products for MLS, developed under the NASA Aura Science Team program. More details on MLS are given in [*Waters et al.*, 2006]. Details of the MLS Level 2 data that the LTDs support are given in [*Livesey et al.*, 2011]. The diagnostics describe the motion of the air masses observed by MLS from 15-days prior to 15-days following each MLS observation. The LTDs are provided to aid scientific studies using MLS observations of atmospheric properties, and are generated for MLS observations from the upper troposphere to the lower mesosphere.

The main files (known as "`combined`" LTDs) contain trajectories running from 15 days prior to 15 days following a "launch day", being a single day of MLS observations. Note that these files represent a "merge" of separate forward and reverse Lagrangian trajectory computations. Accordingly, in these files, the air masses start at some "arbitrary" location 15 days prior to the launch day, pass through a region observed by MLS at the time of that observation on the launch day then travel on a further 15 days. For user convenience, two smaller subsets describe only the launch day and the 5 days either following (`5daysfwd` files) or prior (`5daysrev`).

The LTDs describe diabatic parcel trajectories computed using NASA Global Modeling and Assimilation Office (GMAO) Goddard Earth Observing System (GEOS) model version 5.2 winds and temperature tendencies [*Reinecker et al.*, 2008]. This limits the temporal span of the LTDs to the period from the July 2004 Aura launch to April 30, 2013. Planned updates to the LTD products will use the new GEOS 5.9 record, enabling extension to more recent dates. Parcel advection is computed using a fourth-order Runge Kutta method with a five-minute timestep, based on the algorithm described in *Manney et al.* [1994b].

The specific LTDs described herein are a user-friendly "reduced" subset of a set of "standard" LTD products generated at the MLS Science Computing Facility (SCF). Differences between the reduced and full sets (mainly decreased temporal resolution) are described in section . Some of the quantities within the LTD files, although only relevant for the full files, are retained in the reduced files in order to maintain compatibility and interoperability for user software. A description of all the LTD variables, including these less-relevant ones, is included in this document for completeness.

LTD files and their contents

The LTD file naming convention, is best illustrated by the following example:

```
MLS-Aura_L2LTD-G5D-RedV1p2a_v03-30-c01-ltdv01p0_2005d001-combined.nc
```

In compliance with the Aura-wide file naming convention [*Craig et al.*, 2003] the name consists of four main fields – instrument, product, version, date – separated by underscores, with a file type (`nc`, indicating NetCDF)

following the only period. "Words" within the individual fields are delineated by dashes. The first field, `MLS-Aura`, indicates that this is an Aura MLS product.

The second field, `L2LTD-G5D-RedV1p2a` denotes the product type. `L2LTD` denotes that these are Level 2 Lagrangian Trajectory Diagnostics. `G5D` indicates that the file contains diabatic trajectories (`D`), computed using the GEOS 5.2 wind fields (`G5`). The final word describes the particular trajectory run, with `RedV1p2a` being the current publicly-available run. (the `Red` indicates that these are "reduced" trajectories, as described above; the original "full" trajectories are called `StdV1p2a`).

The third, "version", field mirrors that of the MLS Level 2 data from which the trajectories were launched (e.g., `v03-30-c01`), with additional information on the version of the software used to generate the trajectories (`ltdv01p0`). The final, "date", field gives the Aura format date for the launch day (`2005d001` indicating January 1, 2005), with `-combined` indicating that the file contains a combination of forward and reverse trajectories from 15 days prior to 15 days subsequent to the observations. Alternative smaller files contain only 5-day forward (`5daysfwd`) or reverse (`5daysrev`) trajectory information (though note that the `5daysfwd` file will contain reverse trajectories back to midnight universal time on the launch day, and `5daysrev` forward trajectories to midnight the following day.

The LTD files are stored in the widely used NetCDF format. Each file contains two main sets of information: details of the trajectory launch locations, and information on the motion of each air parcel prior to and following its launch. Table 1 details each quantity in the LTD file and its meaning. The launch information describes, for each trajectory, the latitude, longitude, time and height (actually $-\log_{10}[\text{pressure}/\text{hPa}]$) of its launch, along with arrays relating each launch to a specific MLS profile in the parent MLS Level 2 (L2GP) file.

The trajectory information is simply a set of arrays describing the location (latitude, longitude and potential temperature, stored as $\log_{10}[\theta/\text{K}]$) of each air parcel at each timestep. In addition to location and local atmospheric temperature, additional information can be stored for each trajectory in fields prefixed with `extra_`. Currently only potential vorticity (SPV, scaled as in *Manney et al.* [1994a]), equivalent latitude [*Butchart and Remsberg*, 1986] derived from the SPV, and a diagnostic of trajectory dispersion are so stored; others may be added later. Units for all fields are described in the supporting metadata. All latitudes, longitudes and equivalent latitudes are in degrees, temperatures are in Kelvin, and distances are in meters. Times are given in the EOS-standard "TAI93" format, being the number of seconds since midnight universal time on January 1, 1993 (including the subsequent leap seconds). Other units are given in table 1.

The large arrays associated with the trajectory information are stored "packed" (i.e., as scaled and offsetted two-byte integers). The required unpacking is handled transparently to the user by some NetCDF reading software (e.g., Matlab) but not others (most notably IDL where the user has to apply the offset and scaling themselves). The quantization imposed by this storage equates to ~500 m horizontal and ~1.5 m vertical accuracy.

Obtaining the LTD files

The LTD files are available by anonymous FTP from the MLS Science Computing Facility (SCF) at

`ftp://mls.jpl.nasa.gov/pub/outgoing/ltd/`

Within the FTP repository, all files are currently in the `G5D-RedV1p2a` directory, under which are subdirectories containing the `combined`, `5daysfwd` and `5daysrev` collections, each of which is further grouped in subdirectories for each year.

People are encouraged to register as an LTD user, in order to be kept informed of updates and other issues. The registration page is at `http://mls.jpl.nasa.gov/forms/regltd.php`. In addition, the MLS team would appreciate being informed (via an Email to `data@mls.jpl.nasa.gov`) of any publications using the LTD products.

Table 1: Contents of the LTD files

Name	Type	Describes	Dimensions	Description
LTDVersion	Attribute	File	—	Version identifier for LTD file format (v1.0 currently).
LTDFormat	Attribute	File	—	Indicates LTD file format, usually set to Compact to indicate the use of packed 2-byte integer storage for trajectory arrays.
Unfinished	Attribute	File	—	Used during production to spot cases where file generation crashed etc. Should be set to zero.
LaunchCoordinate	Attribute	Launches	—-	Set to P to indicate that the trajectories are launched at fixed pressures.
TrajectoryType	Attribute	Trajectories	—	Set to D for Diabatic (or I for Isentropic).
time0	Attribute	Trajectories	—	TAI93 format time (seconds since January 1, 1993) for first timestep in file.
startTime	Attribute	Trajectories	—	String format time (Aura format date followed by time) for first timestep in file.
dTime	Attribute	Trajectories	—	Time (in seconds) between output timesteps in the trajectory arrays.
trajectory	Dimension	Trajectories & launches	—	Index for arrays with a "trajectory" dimension.
time	Dimension	Trajectories	—	The "timestep" index.
vertical	Dimension	Launches	—	Vertical index for for launch locations (subset of MLS L2GP output pressures).
along	Dimension	Launches	—	An "along-track" index for for launch locations (equates to MLS L2GP profile locations for these LTD files, see below).
across	Dimension	Launches	—	An "across-track" index for for launch locations (not relevant for "reduced" files).
launchHeights	Array	Launches	[vertical]	Launch pressure (stored as $-\log_{10}[p/\mathrm{hPa}]$).
flankingOffsets	Array	Launches	[across]	Indicates initial distance between center and "flanking" trajectories (not relevant in "reduced" files).
launchLevel	Array	Launches	[trajectory]	Index into launchHeights for each launch.
launchAlong	Array	Launches	[trajectory]	"Along track" index for each launch (equates to launchProfile, the MLS L2GP profile index, for these LTD files).
launchAcross	Array	Launches	[trajectory]	"Across track" index for each launch (not relevant for these "reduced" LTDs, always set to zero).
launchProfile	Array	Launches	[trajectory]	MLS Level 2 profile number for each launch (index zero is the first profile in L2GP files for that day).
launchSubProfile	Array	Launches	[trajectory]	Used in cases where trajectories are launched more densely along track than the MLS sampling (not relevant in this case, always set to zero).
launchLat	Array	Launches	[trajectory]	Latitude of each launch (degrees).
launchLon	Array	Launches	[trajectory]	Longitude of each launch (degrees).
launchTime	Array	Launches	[trajectory]	Time of each launch in TAI93 (seconds since January 1, 1993) format.
times	Array	Trajectories	[time]	Time for each output timestep (TAI93 format).
lat†	Array	Trajectories	[trajectory, time]	Latitude of each trajectory at a given timestep.
lon†	Array	Trajectories	[trajectory, time]	Longitude of each trajectory at a given timestep.
z†	Array	Trajectories	[trajectory, time]	Potential temperature of each trajectory at a given timestep ($\log_{10}[\theta/\mathrm{K}]$).
temperature†	Array	Trajectories	[trajectory, time]	Atmospheric temperature (in Kelvin) of each trajectory at a given timestep.
extra_eql†	Array	Trajectories	[trajectory, time]	Equivalent latitude of each trajectory at a given timestep.
extra_spv†	Array	Trajectories	[trajectory, time]	Scaled potential vorticity of each trajectory at a given timestep.
extra_-flankseparation†	Array	Trajectories	[trajectory, time]	Distance (in meters) between the trajectory and its "flanking" trajectory at a given timestep.

† Denotes arrays stored as packed (scaled and offset) 2-byte integers.

Notes on "reduced" vs. "standard" trajectories and other issues

These "reduced" LTD products described here require ~250 Gb of storage per year of MLS observations for the `combined` set, with ~50 Gb per year for each of the `5daysfwd` and `5daysrev` sets. These are all derived from a significantly more voluminous record of "standard" LTDs that require 2.1 Tb per year. Differences between standard and reduced LTDs are twofold. Firstly, standard LTDs record the parcel location every 20 minutes rather than every two hours. Secondly, standard LTDs actually describe two sets of trajectories. One set is launched from along the MLS track, as for the reduced LTDs, the other set is launched 20 km to the right of the MLS track (i.e., to the east for ascending parts of the orbit and to the west for descending). The divergence of each parcel pair is one measure of the reliability of the trajectory calculation. The reduced LTDs retain the locations of only the "along track" parcels, but also contain an additional field (`extra_flankseparation`) that records the distance (in meters) between the two "parallel" trajectories at each output time.

Although the `launchTime` field denotes the TAI93-format time of each launch (i.e., each MLS profile observation), the actual effective trajectory launch times are rounded to the nearest 20-minute timestep. Note that, unless that timestep coincides with one of the two-hour timesteps in the reduced files, the trajectory will not be "seen" to land directly on the MLS observation location (as recorded in `launchLat` and `launchLon`). In any case, even for those that are launched 10 minutes either side of a two-hour timestep, the quantization introduced by the two-byte integer storage means that `lat` and `lon` will likely not coincide exactly with `launchLat` and `launchLon`.

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References

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